

A Quantum Mechanic Picture

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Abstract On this paper I present a quantum representation based on linear momentum, which is independent of wave function. I derived one equation that relates external potential with linear momentum and other that allows calculate wave function through it. The first one is a non homogeneous first order differential equation and the second one demands uniquely to evaluate an integral. Throughout this paper, I solve two systems using this methodology in order to demonstrate its feasibility. Since it is necessary obtain in first place momentum, a change on focus from wave function to momentum is given. It is not a novelty on quantum applied methods a change of variable, and the experience shows that some advantages can arise with it, so it is reasonably to expect an unfolding of new methods based on our representation.

Keywords Linear momentum · Direct calculation · New methodology

1 Introduction

Quantum mechanics has wave function(Ψ) as its core variable, for which all properties of any system are obtained. It is calculated using Schroedinger equation(equation 1)[1]. However, it is not the only way to work on these problems. The most famous change of variable is made on the Density Functional Theory (DFT) [2,3] that takes electronic density($\rho(x)$) as main variable. DFT is aimed to solve multi-electronic systems by mapping this problem in a single electron one. In analogy to the idea of changing variables, I present here an initial development of a representation that places linear momentum(ζ) as a fundamental variable for quantum systems. Differently of $\rho(x)$ which is derived from wave function, ζ actually has to be calculated before ψ . Although a

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change of variable is not itself a guarantee of a better way for solving problems, we expect that our representation could bring a new way to address them.

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x, y, z) + U(x, y, z)\psi(x, y, z) = E\psi(x, y, z) \quad (1)$$

2 Deriving

I start by writing partial derivatives of wave functions, which are actually the definition of momentum operator:

$$\frac{\partial\psi(x, y, z)}{\partial x} = \zeta_x(x, y, z)\psi(x, y, z) \quad (2)$$

$$\frac{\partial\psi(x, y, z)}{\partial y} = \zeta_y(x, y, z)\psi(x, y, z) \quad (3)$$

$$\frac{\partial\psi(x, y, z)}{\partial z} = \zeta_z(x, y, z)\psi(x, y, z) \quad (4)$$

where ζ differs from linear momentum by a constant: $\zeta_{x_i} = \frac{i}{\hbar}p_{x_i}$. All three relationships (2, 3 and 4) above can be differentiated again so that:

$$\frac{\partial^2\psi(x, y, z)}{\partial x_i^2} = \frac{\partial\zeta_{x_i}}{\partial x_i}\psi(x, y, z) + \zeta_{x_i}(x, y, z)\frac{\partial\psi(x, y, z)}{\partial x_i} \quad (5)$$

Replacing single partial derivatives found on equations 2, 3 and 4 and summing on all directions we have:

$$\sum_i \frac{\partial^2\psi(x, y, z)}{\partial x_i^2} = \sum_i \frac{\partial\zeta_{x_i}}{\partial x_i}\psi(x, y, z) + \sum_i \zeta_{x_i}^2(x, y, z)\psi(x, y, z) \quad (6)$$

Laplacian on the left side can be replaced by Schroedinger equation:

$$-\frac{2m(E - U)}{\hbar^2} = \nabla \cdot \zeta + |\zeta|^2 \quad (7)$$

Equation 7 is part of the set of equations on this methodology. A second one is obtained by solving equations 2, 3 and 4:

$$\psi(x, y, z) = Ae^{\int \zeta \cdot d\mathbf{r}} \quad (8)$$

Also, since commutator of P_x and P_y is zero, any pair of coordinates will be related as follows:

$$\frac{\partial\zeta_{x_i}}{\partial x_j} - \frac{\partial\zeta_{x_j}}{\partial x_i} = 0 \quad (9)$$

This will result on:

$$\nabla \times \zeta = 0 \quad (10)$$

Integrating equation 7 on a volume and applying divergence theorem we obtain:

$$\oint \zeta \cdot \hat{n} dS = - \int \zeta^2 dV - \int \frac{2m(E - U)}{\hbar^2} dV \quad (11)$$

choosing a small finite interval of integration (a cylinder with small lids and side surface infinitesimally small):

$$\zeta_n = \zeta_n^0 - \zeta^2 \delta x_n - \frac{2m(E - U)}{\hbar^2} \delta x_n \quad (12)$$

where n stands for normal direction. Also, a zero curl field yields, after applying Stokes theorem, a continuous tangent component of ζ :

$$\zeta_t = \zeta_t^0 \quad (13)$$

Equations 12 and 13 allows calculation of ζ directly and, consequently, wave function as well. This constitutes an achievement on this representation.

It is worthy mention that this pictures renders a classic-like equation for energy. Rearranging equation 7 we find:

$$E = -\frac{\hbar^2}{2m} |\zeta|^2 + U - \frac{\hbar^2}{2m} \nabla \cdot \zeta \quad (14)$$

Equation 14 displays a hamiltonian for a single point on space with potential given by $V = U - \frac{\hbar^2}{2m} \nabla \cdot \zeta$. Such relation can be interpreted as a classic particle which combined with infinity others form the wave function. They evolve on time accordingly to a force obtained with V .

Following, some well known potentials[4] are solved here in order to demonstrate the method.

2.1 Free Particle.

On this case, potential(U) and ζ are constant, so $\nabla \cdot \zeta = 0$:

$$\zeta = \pm i \frac{\sqrt{2m(E - U_0)}}{\hbar} \quad (15)$$

As ζ can be either positive or negative, solution is made of a linear combination taking both. Also, solving in one dimension:

$$\psi(x) = C \exp\left(i \frac{\sqrt{2m(E - U_0)}}{\hbar} x\right) + D \exp\left(-i \frac{\sqrt{2m(E - U_0)}}{\hbar} x\right) \quad (16)$$

Table 1 Solutions for energy and phase velocity for quantum oscillator system

Energy	velocity
$E_0 = \frac{\hbar\omega}{2}$	$\zeta_0(x) = -\frac{m\omega x}{\hbar}$
$E_1 = \frac{3\hbar\omega}{2}$	$\zeta_1(x) = \frac{1}{x} - \frac{m\omega x}{\hbar}$
\vdots	\vdots

Now, we place the particle in a quantum well with $U = 0$ inside it and limited by an infinity potential on $x = 0$ and $x = a$. The solution is now rewritten as:

$$\psi(x) = F \cos\left(\frac{\sqrt{2mE}}{\hbar}x\right) + G \sin\left(\frac{\sqrt{2mE}}{\hbar}x\right) \quad (17)$$

as we know this wave function must be zero on borders of the well, so $x = 0$ makes $F = 0$ and $x = a$ makes $\frac{\sqrt{2mE}}{\hbar}a = n\pi$, yielding the well known energy states:

$$E = \frac{n^2\hbar^2}{8m\pi^2a^2} \quad (18)$$

2.2 Harmonic Oscillator.

External potential on this system is given by $U = m\omega^2x^2/2$. Placing it on equation 7, we found the set of energy eigenvalues and ζ shown on table 1.

3 Numeric solution: Hydrogen atom

I restrict this solution for one dimensional case, so $\zeta_t = 0$ and equation 12 will be written as:

$$\zeta(x + \delta x) = \zeta(x) - \zeta(x)^2\delta x - \frac{2m(E - U(x))}{\hbar^2}\delta x \quad (19)$$

The solution for ζ calculated for the third energy level is shown on figure 1. Also wave function for three initial energy states are displayed on figure 2.

4 conclusion

I presented on this paper a new representation for quantum mechanic calculation based on wave function momentum. As result, three equations (7, 8 and 10) were derived, relating ζ directly with external potential U and relating wave function with ζ . Also, as result a direct way of calculating wave function is obtained.

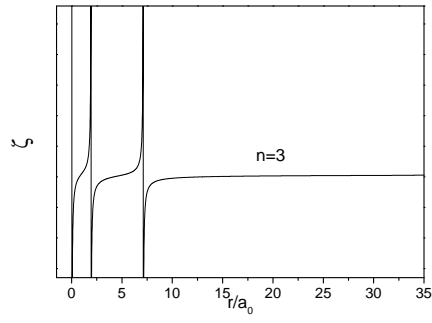


Fig. 1 Phase velocity calculated for third energy level.

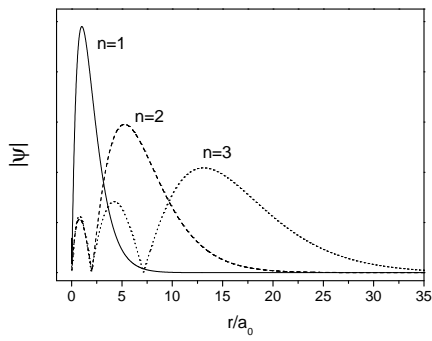


Fig. 2 Wave function module for hydrogen atom calculated for first three initial states.

References

1. Schrödinger, E. *Phys. Rev.* **28**, 1049–1070 Dec (1926).
2. Hohenberg, P. and Kohn, W. *Phys. Rev.* **136**, B864–B871 Nov (1964).
3. Kohn, W. and Sham, L. J. *Phys. Rev.* **140**, A1133–A1138 Nov (1965).
4. Eisberg, R., Resnick, R., and Brown, J. *Quantum physics of atoms, molecules, solids, nuclei, and particles*, volume 39. (1986).